

Molecular Dynamics News

number 89, June 1997

MDN is an informal newsletter of coming attractions and current events in the world of reaction dynamics and associated phenomena. It is produced without profit through the support of its subscribers* and patrons. Please renew your subscription by using the form at the bottom of this page.

The format for MDN is

- a Announcements of *open positions* (faculty and postdoctoral).
- b Information about *papers*, whether accepted or not, which are available for distribution. Please state in separate lines: *Title. Journal* (If ms. has been accepted - otherwise state *unpublished*). *Author(s). Address.* (Star author to whom correspondence should be addressed and whose mailing address is given.) In a separate final line provide a *one-sentence punch line*. Please follow this format.
- c Announcements of *conferences, topical meetings, etc.* Availability of *special materials* (e.g., annual reports, computer programs, experimental designs and tips, etc.). *Progress* (or activity) *reports* about work which is not yet published but which may be of interest to our community.
- d Electronic mail addresses and FAX numbers.

MDN is edited by Prof. Vincenzo Aquilanti, Dipartimento di Chimica dell' Università, 06123 Perugia, Italy (electronic mail: AQUILA@HERMES.CHM.UNIPG.IT) and Prof. Roger W. Anderson, Dept. of Chemistry, University of California, Santa Cruz, CA 95064, U.S.A. (electronic mail: ANDERSO@CATS.UCSC.EDU).

Send all material for issue 90 to Prof. R. Anderson (You are encouraged to use electronic mail: ANDERSO@CATS.UCSC.EDU). (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#89). The closing date for issue number 90 is August 1, 1997.

*1997 Calendar-Year subscription for MDN, (six issues).

North America: (\$20/year US currency) : Your check for one or more years should be paid out to The Regents of the University of California. Send it to Roger W. Anderson, and include your name, address, and optional information like email addresses and FAX numbers.

Elsewhere: Your check for the equivalent of US \$20/year in any convertible currency should be paid out and sent to Prof. V. Aquilanti. **Amount enclosed**

Name: _____
Address: _____

Electronic Mail Address (optional): _____

WWW Address (optional): _____

Fax Number (optional): _____

Delivery Method: Hardcopy _____ Email(PostScript) _____ Email(LaTeX) _____ Mosaic _____

ANNOUNCING ELECTRONIC DELIVERY OF MDN

We offer to our subscribers several possibilities for electronic delivery of MDN:

1. Electronic mail to subscribers

In this case subscribers tell us if they want the newsletter automatically sent to them by electronic mail. The newsletter can be sent in two forms: raw LaTeX source file, or as a Postscript file. Subscribers may specify the desired form.

2. World Wide Web

Now anyone can access the newsletter as a LaTeX, dvi, HTML, pdf or Postscript file. A Web browser such as Mosaic or Netscape with suitable viewers allows people to read the files on their computer screens. Alternatively the files can be downloaded for local viewing or printing. Subscribers choosing this delivery option will receive an email announcement when a new issue is posted. For information you are welcome to visit the Molecular Dynamics News World Wide Web site:

<http://www.ucsc.edu/mdn>

We periodically update the home page, and you can find links to Molecular Dynamics News subscribers' home pages at our WWW site. We will add a link to your home page if you send us the address by email or with the subscription form on the cover page of this issue. There is also a list of MDN subscribers that is linked to their email addresses.

We appreciate electronic mail with your reactions to this proposal and with updated email addresses. Please send your email messages to MDN@CHEMISTRY.UCSC.EDU

We continue to send hardcopy newsletters by mail to subscribers who request this form of delivery.

The MDN e-mail list continues, as detailed below

MOLECULAR DYNAMICS NEWS EMAIL LIST

All members of the chemical physics community are invited to join the (free) "molecular-dynamics-news" email list. The "molecular dynamics" in the title is to be interpreted as meaning "dynamical processes in molecules" rather than "classical simulations of molecular motion". The list can be used to distribute details of conferences, vacant academic and postdoctoral positions, changes of address and other news in the Molecular Dynamics field. It also serves as an archive of up-to-date email addresses for people in the field. The list was created by Jeremy Hutson in June 1993 and in January 1997 has about 1300 members. Instead of being maintained manually, the list is operated by a system called "mailbase". People can join or leave the list simply by sending messages to the mailbase program, without the list owner needing to do anything. To join the email list, send a message to the Internet address mailbase@mailbase.ac.uk containing a line of the form:

join molecular-dynamics-news John F Kennedy

You do not need to tell the program your email address, as it picks it up from the message header. It does need to be told your real name, so that it can maintain a useful list of email addresses.

When you join, you will receive some introductory information on how to circulate information to the molecular-dynamics-news list, and on the mailbase system itself.

If you would like a list of the current members, send a message containing the line
review molecular-dynamics-news
to the address mailbase@mailbase.ac.uk

Note that messages distributed via the e-mail list are not normally printed in the newsletter, unless the Editors receive an explicit request to do so.

There is also a spectroscopy email list. To join this email list, send a message to the Internet address mailbase@mailbase.ac.uk containing a line of the form:

join spectroscopy-group John Kennedy

a. Open Positions

FACULTY

BEN-GURION UNIVERSITY OF THE NEGEV, ISRAEL

The Chemistry Department of Ben-Gurion University of the Negev seeks outstanding candidates for a tenure track faculty position. Field of interest is open. Applicants with Ph.D obtained within the last 7 years should send current CV, outline of research interests and plans, and names of at least three references to Prof. James Y. Becker, Chair, Chemistry Department, Ben-Gurion University of the Negev, Beer Sheva, Israel 84120. Teaching in Hebrew is expected within three years. Deadline for applications is 6.30.97.

POST DOCTORAL AND VISITING

NATIONAL TSING HUA UNIVERSITY, DEPARTMENT OF CHEMISTRY

Two postdoctoral positions starting August 1, 1997 (flexible) at the Department of Chemistry, National Tsing Hua University, TAIWAN. Possible projects include: (1) Two-color resonant four-wave mixing spectroscopy of free radicals in a supersonic jet, (2) Time-resolved Fourier-transform Spectroscopy with a step-scan FTIR - spectroscopy, kinetics, and dynamics after laser photolysis of gaseous molecules. (3) Photoionization spectroscopy and kinetic of free radicals using synchrotron radiation source or VUV laser. Extended experiences with excimer and Nd-YAG lasers preferred. Good salary with yearly renewable appointment. Applicants should arrange 2-3 letters of recommendation to be sent to Prof. Y. P. Lee, I-C. CChen, Department of Chemistry, National Tsing Hua University, TAIWAN 30043 (e-mail: yplee@net.nthu.edu.tw, icchen@net.nthu.edu.tw, FAX: 886-3-5722892).

CENTER FOR MOLECULAR REACTION DYNAMICS AND LASER CHEMISTRY, DENMARK

A number of postdoc positions or postdoc-like guest positions of one year duration, starting 1997 are open. The center consists of a group of scientists from different institutions in Denmark, representing both theoretical and experimental activities.

THEORY: The theoretical groups are the following:

Gert Due Billing (University of Copenhagen), Carl Nyeland (University of Copenhagen), Niels Engholm Henriksen (Technical University, Copenhagen), Flemming Yssing Hansen (Technical University, Copenhagen), Frank Jensen (Odense University), Kurt V. Mikkelsen (University of Copenhagen), Ole Sonnich Mortensen (Odense University)

The present theoretical activities are concentrated within the topics chemical reactions, photodissociation, laser induced processes, electron-proton transfer, reactions in solution, electronic structure calculations, semiclassical reactions, control of chemical reactions, transport properties etc. The theoretical methods applied range from classical statistical mechanics to full scale quantum mechanical dynamics.

EXPERIMENT: The experimental groups are the following:

Robert Wilbrandt (Riso National Laboratory), Soren Rud Keiding (University of Aarhus), Nis Bjerre (University of Aarhus)

The present experimental activities are concentrated within the areas time-resolved optical spectroscopy and high-resolution spectroscopy, in particular structural and dynamical investigations of chemical intermediates in condensed phase by laser flash photolysis, resonance Raman scattering and quantum chemical calculations; ultrafast laser spectroscopy and high resolution spectroscopy in molecular beams, THz-pulses and coherent control.

Salary according to guidelines for the University in question.

Potential applicants should contact

Prof. Gert Due Billing, tlf. +45 35320252 E-mail: gdb@moldyn.ki.ku.dk

Dr. Robert Wilbrandt, tlf. +45 46774248 E-mail: WILBRANDT@risoe.dk

Assoc. Professor Kurt V. Mikkelsen, tlf. +45 35320251 E-mail: kmi@teosgi2.ki.ku.dk

Assoc. Professor Niels Engholm Henriksen, tlf. +45 45252029 E-mail: neh@tkemi.klb.dtu.dk
Assoc. Professor Frank Jensen, tlf. +45 66158696-2507 E-mail: frj@dou.dk
Assoc. Professor Soren Rud Keiding, tlf. +45 89483333 E-mail: keiding@kemi.aau.dk
Formal application including a CV, list of publications and research areas of interest should be submitted in 5 copies by May 15'th to
Prof. Gert Due Billing, H. C. Oersted Institutet, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark
Fax: +45 35320259

NORTHWESTERN UNIVERSITY, DEPARTMENT OF CHEMISTRY

I am looking for a theory postdoc to help me with a new project that falls at the interface of optical physics and materials chemistry. This is a collaborative project which involves my colleague Mark Ratner as well as several experimentalists (R. Van Duyne, J. Hupp, W. DeHeer, M. Jarrold, C. Mirkin, J. Ketterson), and the primary activity for this position is to develop and apply theories which are capable of describing the optical properties, both linear and nonlinear, of assemblies of clusters or nanoparticles. This would be an ideal position for someone with interests in light scattering theory and/or nonlinear optics, but I am willing to be flexible. There is also a connection with magnetic nanoparticles, so background in the magnetic properties of materials is another possibility. Some of our work would build on past studies in my lab of absorption spectra and Raman intensities using converged electrodynamics calculations. References to this past work are: W. -H. Yang, G. C. Schatz and R. P. Van Duyne, JCP 103, 869 (1995); W. -H. Yang, J. Hulteen, G. C. Schatz and R. P. Van Duyne, JCP 104, 4313 (1996) and A. C. R. Pipino, R. P. Van Duyne and G. C. Schatz, Phys. Rev. B53, 4162 (1996).

The position is available May 1, but a later starting date is possible.

Interested applicants should send their resume and two letters of recommendation to:

Prof. George C. Schatz, Department of Chemistry, Northwestern University, Evanston, IL 60208-3113

NATIONAL RESEARCH COUNCIL, STEACIE INSTITUTE

I am looking for a postdoctoral fellow to work with me on problems in theoretical physics or chemistry. My research interests include the interaction of molecules with intense fields, chemistry and photochemistry at interfaces, mathematical method development and condensed-phase dynamics.

The Steacie Institute of the National Research Council is located in downtown Ottawa, next to the Ottawa River. The annual salary is about \$40,000 CAN, commensurate with experience.

For more information please see <http://gold.nrc.ca/tamar> or contact me by phone, e-mail or Fax.

Tamar Seideman, Steacie Institute of Molecular Science, National Research Council of Canada, Ottawa K1A 0R6

Tel: 613-990-0945, e-mail: tamar.seideman@nrc.ca, Fax: 613-954-5242

INSTITUTE FOR MOLECULAR SCIENCE

Applications are invited for a postdoctoral position in the research group of Prof. Toshinori Suzuki at Institute for Molecular Science, Okazaki, Japan. The current research projects involve studies of photodissociation and reactive scattering of polyatomic molecules. Reaction dynamics is studied by state-resolved speed, angular, and alignment distributions of products and their time-evolution. Molecular beam methods are coupled with 2D ion imaging with nanosecond or femtosecond lasers. Interested candidates should send a CV and the names of two or three references to Toshinori Suzuki, Institute for Molecular Science, Myodaiji, Okazaki 444 Japan (e-mail suzuki@ims.ac.jp, FAX +81-564-54-2254)

CORNELL UNIVERSITY, Department of Chemistry

Two postdoctoral positions are available to work in the general area of photodissociation dynamics in the laboratory of Paul Houston at Cornell University. Successful applicants should have had significant

experience with pulsed nanosecond dye lasers and, if possible, with pulsed molecular beams. One position is to investigate the photodissociation dynamics of ozone using photofragment imaging and Rydberg time-of-flight techniques. One position is to investigate the photodissociation dynamics of radical species. Descriptions of the current research group and recently completed projects can be found on the web: <http://www.msc.cornell.edu/plh2/group>

Applicants should send a curriculum vitae and arrange for letters from three references to be sent to Paul L. Houston, Department of Chemistry, Cornell University, Ithaca, New York 14850-1301 USA.

UNIVERSITY OF BRITISH COLUMBIA, THEORETICAL CHEMISTRY

A postdoctoral position in theoretical chemistry is available immediately in the group of Mark Thachuk for a period of one year, with an option to renew for a second year if mutually desirable. Areas of research include the interaction of molecular ions with intense laser fields, time-dependent semi-classical hopping methods, and gas phase reaction dynamics. Salary is within NSERC guidelines.

The University of British Columbia is located in the beautiful port city of Vancouver, nestled in the Rocky mountains with wonderful skiing and hiking nearby.

Interested applicants please send a curriculum vitae, and arrange for three letters of reference to be sent to: Mark Thachuk, Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, BC, Canada V6T 1Z1

Email: thachuk@chem.ubc.ca, Tel: (604) 822-2448, FAX: (604) 822-2847

Information about the Chemistry Department is available on the web at <http://www.science.ubc.ca/departments/chem>.

IOWA STATE UNIVERSITY, DEPARTMENT OF CHEMISTRY

Postdoctoral positions are available summer or fall 1997 at salary: \$30,000/year. The applicants must have a physics or chemistry Ph.D., or related area after January 1994, with excellent background in fundamental quantum mechanics and electronic structure theory

The general goals of this research are to develop and apply new variational one-electron density functional theories that will allow direct computation of interaction potentials and forces in large complex systems. For more information, see <http://aztec.fi.ameslab.gov:80/depristo/>.

One can also work in two other areas: Cluster Structure and Reactivity and Thin film growth.

Applications must include: resume, publication list, unofficial photocopies of undergraduate and graduate transcripts, three letters of reference, a detailed description of your computer experience on PC's, workstations, vector and parallel supercomputers in 1 page or less, noting program, operating system and language expertise.

Send the above information to: Professor Andrew E. DePristo, 303 Wilhelm Hall, Ames Laboratory, Iowa State University, Ames, IA 50011. (e-mail to depristo@ameslab.gov for documents using MIME compliant mailers.)

Ames Lab and Iowa State University are equal opportunity employers.

ACADEMIA SINICA, INSTITUTE OF ATOMIC AND MOLECULAR SCIENCES

A post-doctoral position is open in the group of Prof. Y.T. Lee at the Institute of Molecular Sciences (IAMS) of Academia Sinica, Taiwan, ROC, in the field of chemical reaction dynamics. Over the past three years, we have employed the crossed molecular beams technique to elucidate the chemical dynamics, energetics, and reaction products of C(3Pj) reactions with unsaturated hydrocarbons and hydrogen sulfide in extraterrestrial environments. Our investigations revealed that these atom-neutral reactions established a versatile route to form carbon-containing radicals in the interstellar medium (dark clouds and outflow of dying carbon stars), in atmospheres of Jupiter, Saturn and its moon Titan, Uranus, as well as Neptune, and after impact of comet Shoemaker-Levy 9 into the Jovian atmosphere. The prime directive of the new candidate is to extend these studies to explore the chemical dynamics of reactions involving boron and silicon atoms with closed shell

molecules employing the crossed molecular beams technique. Energetic candidates should send inquiries prior to September 1, 1997 to:

Dr. Ralf-I. Kaiser, Department of Chemistry, University of California, Berkeley CA 94720, tel: 510-4865741, fax: 510-4865311, email: kaiser@leea.cchem.berkeley.edu

UNIVERSITY OF COIMBRA

A postdoctoral research position is available in Theoretical & Computational Chemistry at the Group of Professor A. J. C. Varandas. The position is for research on potential energy surfaces and reaction dynamics, with emphasis on systems with relevance in atmospheric chemistry and combustion processes. Applicants are sought with good experience on the ab initio calculation of potential energy surfaces and/or reaction dynamics. The position is initially for one year, with renewal depending on mutual agreement. Applicants are welcome from all nationals who have obtained a PhD, with the position being available from September 1997. A later starting is negotiable. Interested candidates should submit a curriculum vitae, and arrange for two or three letters of recommendation to be sent to:

Professor A. J. C. Varandas, Departamento de Química, Universidade de Coimbra, 3049 Coimbra Codex, Portugal.

For further information please contact Professor A. J. C. Varandas via e-mail:

VARANDAS@GEMINI.CI.UC.PT; telephone: 351-39-35867; fax:351-39-27703

b. Preprints

Quasiclassical trajectory study of molecular alignment effects on the dynamics of the reactions of Cl, Br and I with H₂.

J. Phys. Chem. (submitted)

Miguel Gonzalez (a), J. D. Sierra (b), R. Francia (b), and R. Sayos (a)

(a) Departament de Quimica Fisica, Universitat de Barcelona, Marti i Franques, 1.08028 Barcelona, Spain;

(b) Departamento de Quimica, Universidad de La Rioja, Obispo Bustamante, 3. 26001 Logroño, Spain

The title reactions may be taken as models for endoergic triatomic reactions with heavy-light-light kinematics and collinear saddle point. The dependence of scalar and two-vector properties on reactants conditions (ET, v, j), as well as the effect of considering initial parallel, perpendicular and random k-j alignment has been studied.

Two-Center Coulomb Functions

Comp. Phys. Comm., submitted.

Miyabi Hiyama and Hiroki Nakamura*

Dept. Theo. Studies, Inst. for Molec. Sci.

Myodaiji, Okazaki 444 Japan.

Code to numerically evaluate two-center Coulomb functions.

Gaussian Expansions of the Two-Center Coulomb Functions

Comp. Phys. Comm.

Miyabi Hiyama and Hiroki Nakamura*

Dept. Theor. Studies,

Inst. for Molec. Sci.

Myodaiji, Okazaki 444, Japan.

Conventional CI code can be used to evaluate electronic transition matrix element involving two-center Coulomb functions.

Nonadiabatic Transitions at Potential Curve Crossings and a New Mechanism of Molecular Switching.

J. Korean Physical Society

Hiroki Nakamura

Dept. Theor. Studies

Inst. for Molec. Sci.

Myodaiji, Okazaki 444, Japan.

New theory for the Landau-Zener-Stueckelberg problems is reviewed, molecular switching based on the complete reflection phenomenon.

Chemical Reaction Dynamics and Potential Ridge—Beyond Transition State.

In The transition State—A theoretical Approach, edited by T. Fueno (Kohdansha and John Wiley & Sons, 1997)

Hiroki Nakamura

Dept. Theor. Studies,

Inst. for Molec. Sci.

Myodaiji, Okazaki 444, Japan.

Theoretical Studies of Chemical Dynamics: Overview of Some Fundamental Mechanisms.

Ann. Rev. Phys. Chem. vol. 48, 1997.

Hiroki Nakamura

Dept. Theor. Studies,

Inst. for Molec. Sci.

Myodaiji, Okazaki 444, Japan.

Vapor Grown Polycrystalline Diamond Films: Microscopic, Mesoscopic and Atomic Surface Structures

submitted

H.-G. Busmann# and I.V. Hertel*

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy

Postfach 1107, 12474 Berlin, Germany

#Fraunhofer-Institut fuer Angewandte Materialforschung (IFAM,) Lesumer

Heerstrasse 36, D-28717 Bremen, Germany

A detailed analysis with scanning electron and electron tunneling microscopy of microscopic, mesoscopic, and atomic surface structures as well as the growth forms of vapor grown polycrystalline diamond films is presented. The growth form as a function of the substrate temperature T_s shifts from the octahedral shape at 990 K over the cubo-octahedral shape at 1100 K to the cubic shape at 1275 K.

Cluster size dependence of the internal conversion in highly excited benzene(NH₃)_n clusters.

Chemical Physics Letters 264 (1997) 210-214

W. Radloff, Th. Freudenberg, V. Stert, H.-H. Ritze, F. Noack and I.V. Hertel

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy,

Postfach 1107, 12474 Berlin, Germany

The size dependence of the internal conversion efficiency for the optically excited electronic S_2 -state in benzene(NH₃)_n clusters has been studied. The analysis of pump-probe experiments with 160 fs laser pulses reveals a significant enhancement of the S_2 to S_1 conversion probability with the number n of ammonia molecules in the cluster. In contrast, the total deactivation rate of the S_2 -state by internal conversion of about 10^{-13} s^{-1} is nearly independent of the cluster size.

Pulse-width influence on laser structuring of dielectrics.

Nuclear Instruments and Methods in Physics Research B 122 (1997) 359-363

D. Ashkenasi, H. Varel, A. Rosenfeld, F. Noack, E.E.B. Campbell

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107,
12474 Berlin, Germany

The morphology of several dielectrics (α -SiO₂, CaF₂ and BaF₂) irradiated by laser light at a wavelength of 790 nm for different pulse width (between 200 fs and 5 ps) and fluences near the single shot damage threshold has been investigated by using the complementary techniques of electron microscopy and atomic force microscopy. Differences can be observed which we relate to the mechanisms and dynamics of defect production in these wide bands gap materials.

IR Spectroscopy and HPLC Separation of Endohedral Li@C₆₀

Proceedings Kirchberg, 1997

N. Krawez*, R. Tellgmann*, A. Gromov#, W. Kraetschmer# and E.E.B. Campbell*

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107,
12474 Berlin, Germany

Max Planck Institut fuer Kernphysik, Postfach 193980, D-69029 Heidelberg

The infrared spectroscopy of thin films of fullerenes containing approximately 30% endohedral Li@C₆₀ has been investigated. A strong signal is observed corresponding to the vibrational motion of the Li inside the fullerene cage. In addition, a number of modes corresponding to the reaction products of the films with air can be observed. The films can be dissolved in CS₂ allowing the chromatographic separation of the pure endohedral material.

Laser Processing of Sapphire with Picosecond and Sub-Picosecond

Appl. Surf. Science, submitted

D. Ashkenasi, A. Rosenfeld, H. Varel, M. Waehmer and E.E.B. Campbell

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107,
12474 Berlin, Germany

Laser processing of sapphire using a Ti:Saph laser at 790 nm and 395 and pulse widths varying between 0.2 and 5ps is reported. A clear improvement in quality is demonstrated for multi-shot processing with sub-ps laser pulses. For fluences between 3 and 12 J/cm² two ablation phases were observed, in agreement with previous work from Tam et al. using 30 ps, 266 nm laser pulsed [1].

The Dispersed Laser Induced Fluorescence Spectrum of Gas Phase C₆₀ at 308 nm

J. Phys. B

St. Firth⁺, P.F. Coheur⁺, R. Mitzner^{*}, M. Carleer⁺, E.E.B. Campbell^{*}, R. Colin¹ and H.W. Kroto¹
⁺Laboratoire de Chimie Physique Moléculaire, Université Libre de Bruxelles-CP 160/09,
50 av. F. D. Roosevelt, 1050-Brussels, Belgium

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107, 12474
Berlin, Germany

¹ School of Chemistry and Molecular Sciences, University of Sussex, Brighton BN1 9QJ, UK

We have recorded the dispersed laser induced fluorescence spectrum of gas phase C₆₀ ablated from a rotating copper cylinder by 308 nm radiation from a XeCl excimer laser. At vibrational energies below 7000 cm⁻¹ the spectrum consists of three progressions of either odd quanta in the lowest frequency t_{2u} mode, with the lowest h_u and g_u modes as additional origins or the third hg mode with two quanta of the lowest gu mode and the combination h_u(1) + g_u(1) as the additional origins. At higher vibrational energies, the observed bands become more complex, and have yet to be analysed.

Vibrational distribution in CN(X²Σ⁺) from the N+C₂ → CN+C reaction.

Chem. Phys.

N. Daugey, A. Bergeat, A. Schuck, P. Caubet and G. Dorthe^{*}.

Laboratoire de Photochimie Moléculaire, Université Bordeaux I, 33405 Talence, France.

A clean source of C₂ radicals allowed to determine the CN(X²Σ⁺) vibrational distribution from the N+C₂ → CN+C reaction in a low-pressure fast-flow reactor.

A crossed molecular beam study of the reaction O(¹D)+HI →IO+H

J. Phys. Chem.

Michele Alagia, Nadia Balucani, Piergiorgio Casavecchia, and Gian Gualberto Volpi

Dipartimento di Chimica dell'Università

Via Elce di Sotto, 8

06123 Perugia, Italy.

Molecular Beam Scattering of Nitrogen Molecules in Supersonic Seeded Beams: a Probe of Rotational Alignment

J. Phys. Chem. Special Issue on Stereodynamics of Chemical Reaction, 1997, accepted for publication.

Vincenzo Aquilanti, Daniela Ascenzi, David Cappelletti, Roberta Fedeli, and Fernando Pirani

Dipartimento di Chimica dell'Università

Via Elce di Sotto, 8

06123 Perugia, Italy.

¹ Istituto per le Tecnologie Chimiche dell'Università

06123 Perugia, Italy.

Total integral cross sections for scattering of nitrogen molecules by Xe atoms in the glory collision energy range are reported, using both a rotationally "hot" effusive beam of nitrogen (obtaining information on the isotropic component of the interaction potential), and rotationally "cold" N₂ seeded beams emerging from supersonic expansions, from which quantitative information on rotational alignment of N₂ are obtained.

Dissociative ionization of methyl chloride and methyl bromide by collision with metastable neon atoms

J. Phys. Chem.

B. Brunetti, P. Candori, J. De Andres[#], and F. Pirani,

Dipartimento di Chimica dell'Università

06123 Perugia, Italy.

M. Rosi, S. Falcinelli, and F. Vecchiocattivi

Istituto per le Tecnologie Chimiche dell'Università

06123 Perugia, Italy.

Exact quantum stereodynamics: the steric effect for the $\text{Li}+\text{HF} \rightarrow \text{LiF}+\text{H}$

J. Chem. Phys.

J. M. Alvarino^{*}, V. Aquilanti, S. Cavalli, S. Crocchianti, A. Laganá, and T. Martínez[#]

Dipartimento di Chimica dell'Università

06123 Perugia, Italy.

^{*} Departamento de Química Física, Universidad de Salamanca,

37008 Salamanca, Spain.

[#] Departamento de Máquinas y Motores Térmicos, Universidad del País Vasco

48012 Bilbao, Spain.

To study the stereodynamics of atom diatom reactions we apply the formalism developed by Aquilanti *et al* (J. Phys. Chem. **95**, 8184 (1991)). As a case study the prototype $\text{Li} + \text{HF} \rightarrow \text{LiF} + \text{H}$ reaction at zero total angular momentum J is considered. For this reaction we calculated the scattering \mathbf{S}^J -matrix in the standard $|lj\rangle$ representation and transformed it into a stereodirected representation. In this way it is possible to investigate the effect on the reaction probability of the orientation of the target HF molecule with respect to Li attack. In the investigated collision energy range (0.45–0.54 eV) propensity is found for Li attack on the side of H-atom.

c. Conferences

1. Optical, electric and magnetic properties of molecules

Cambridge University, UK; 10-13 July 1997.

This conference is being organised to celebrate the career of Professor A. David Buckingham. Those interested in attending should write to Prof. David C Clary, Department of Chemistry, University College London, London WC1H 0AJ, UK or Professor Brian J. Orr, School of Chemistry, Macquarie University, NSW 2109, Australia. The Keynote Lecturers will be: D.P. Craig, N.C. Handy, J.-P. Hansen, D.R. Herschbach, D.A. King, W. Klemperer, R.A. Marcus, J.A. Pople, A.H. Zewail Invited Speakers: L. D. Barron, C. A. de Lange, P. W. Fowler, J. M. Hutson, D. M. Neumark, G. L. D. Ritchie, J.-L. Rivail, R. J. Saykally, P. J. Stephens Principal Organisers: D. C. Clary (UCL, UK) and B. J. Orr (Macquarie, Australia) Conference Secretary: M. J. T. Jordan (Cambridge, UK).

The conference will start after lunch, at 2pm, on Thursday 10 July 1997 and finish with breakfast on Sunday 13 July. Lectures will be held in the Department of Chemistry, University of Cambridge and accommodation will be in Pembroke College Cambridge. Cambridge is easy to get to from London by rail and from Stansted and Heathrow Airports by bus. Sponsors for the conference include Elsevier, Taylor and Francis, Shell and CCP6. The total cost for registration and accommodation will be close to 240 pounds. There will be a limited capacity for contributed poster papers. More details will be sent out in 1997 to those who register their interest now. The www site for the meeting is : <http://nickel.chem.ucl.ac.uk/adb.conference/> If you would like to take part in the conference, please email the form below to: Dr Meredith Jordan, Conference Secretary, Department of Chemistry, University of Cambridge, Lensfield Rd Cambridge, CB2 1EW, UK. Email: mjtj2@cus.cam.ac.uk Fax: [44]-(1223)-336 362

I would like to attend the conference:

OPTICAL, ELECTRIC AND MAGNETIC PROPERTIES OF MOLECULES: A conference to celebrate the career of Professor A. D. Buckingham
July 10-13 1997 Cambridge, UK

Name:

Email:

Fax:

Address:

Suggested Poster Title (optional):

Please email this completed form to mjtj2@cus.cam.ac.uk

2. 1997 Conference on the Dynamics of Molecular Collisions

Gull Lake, Minnesota USA, July 20-25, 1997

The Dynamics of Molecular Collisions (DMC) Conference is the major conference in the United States on the topic of molecular collisions and related phenomena. This conference was begun as a Gordon Conference in 1965, and has been held every two years since then. In recent years it has been held at major resorts around the country, most recently (1995) at the Asilomar Conference Center in Pacific Grove, California (Dan Neumark, chair). The Asilomar Meeting attracted over 300 participants from around the world, with 23 invited talks and about 235 poster talks. The 1997 Conference will be held at Cragun's Resort on Gull Lake near Brainerd Minnesota. This resort is located in the central lakes district of Minnesota in a region of beautiful pine forests and many thousands of lakes. The conference was last held at Cragun's in 1983. Since then the resort has been substantially improved, with increased space for poster and oral talks, modernized sleeping rooms, and many new recreational facilities including an indoor sports center. In addition, Cragun's has its own beach, sail and motor boats, tennis courts and golf course, and nearby are hiking and biking trails and other attractions. Cragun's is about a 2.5 hour drive from the Minneapolis

airport; we plan to arrange for ground transportation to and from the conference. Alternatively, if you fly on Northwest airlines to Minneapolis, the extra fare to fly to the Brainerd airport is about \$40 roundtrip. The scientific program will be international and will cover all aspects of molecular collisions, including reactive and nonreactive collisions, and related photochemistry and surface processes. Both experimental and theoretical topics will be included. Suggestions for specific areas or speakers are welcome and should be addressed to the conference chair. The meeting will follow a Gordon Conference format, i.e., morning and evening sessions from Monday morning to Friday noon, with afternoons free for informal discussions, recreation, and relaxation. Time will be set aside for formal presentation of poster papers and long discussion periods after invited talks. The conference program committee consists of chair George C. Schatz, Northwestern University and vice-chair James J. Valentini, Columbia University. Further details will be announced in the fall of 1996. This conference has generally included at least one representative of almost every major experimental and theoretical group studying molecular collision dynamics in the United States, as well as a very good representation from foreign groups. We hope that you will be able to attend the 1997 meeting and urge you to mark off the week of July 20-25 on your calendar now.

IMPORTANT INFORMATION: If you are interested in receiving additional information concerning this conference (such as the second announcement), please send your name, address, phone, fax and email to: George C. Schatz, Department of Chemistry, Northwestern University, Evanston IL 60208-3113, phone: 1-847-491-5657, fax: 1-847-491-7713, email: dmc@chem.nwu.edu

Web site for conference: <http://www.chem.nwu.edu:80/schatz/index.html> (This web site repeats the information in this announcement right now, but it will eventually contain information about speakers, lists of attendees, information about Cragun's, registration and housing forms, etc.)

3. 1997 TWENTY-THIRD INTERNATIONAL SYMPOSIUM ON FREE RADICALS

Taellberg, Dalarna, Sweden, August 17-22, 1997

Organizing committee:

Mats Larsson (chairman), Physics Department I, KTH, Stockholm (larsson@atom.kth.se)

Bosse Lindgren, Physics Department, Stockholm University, Stockholm

Lars-Erik Berg, Physics Department I, KTH, Stockholm (berg@atom.kth.se)

Sven Mannervik, Atomic Physics, Stockholm University, Stockholm

The 1997 Twenty-third International Symposium on Free Radicals will be held Aug 17- 22, 1997 at Green Hotel, Taellberg, Dalarna, Sweden. The Symposium will address the physical and chemical properties of FREE RADICALS, including paramagnetic molecules, ions, molecules in excited states and short-lived species. A wide variety of topics will be covered by papers and discussions: Spectroscopy of radicals; Dynamics and reaction kinetics, theory and experiment; Structure of free radicals; Molecular ions and molecules in excited states; Free radicals and atmospheric chemistry; Interstellar spectroscopy and chemistry; Free radicals as reaction intermediates; Free radicals in applied research; Production and observation techniques.

There will be several invited talks covering the listed topics above. Contributed papers will be presented in poster sessions with a brief introduction by the author. The conference will be held at Green Hotel, Taellberg near Lake Siljan in Dalarna, Sweden. It is located 280 km from Stockholm. Taellberg is easy accessible from Stockholm (3 1/2 hours by train or car, 40 min by flight to Dala airport and then car transportation). This part of Dalarna is one of the most attractive tourist sites in Sweden. There are many activities and places of interest around Lake Siljan. Further information can soon be obtained from the conference home page on <http://www.atom.kth.se>

4. CONDENSED PHASE QUANTUM DYNAMICS: APPLICATION TO CHEMICAL AND BIOLOGICAL SYSTEMS

Lausanne, Switzerland 28-30 August 1997

Chairpersons: Prof. M. Chergui and Dr M. T. Portella-Oberli

The scientific programme of this meeting will emphasize the various aspects of condensed phase dynamics as probed by conventional and ultrafast laser techniques. The topics that will be covered during the meeting include photoinduced dynamics in solids and liquids, interfaces and surfaces, biological molecules and polymers. Contributions, by both experimentalists and theoreticians, will be made to an audience of not more than 80 people. This format will allow intense discussions and a fruitful exchange of ideas. A poster session is also planned. This conference precedes the Femtochemistry Conference in Lund (1-4/9/1997)

Speakers that have confirmed participation include: A. H. Zewail (USA), V.S. Letokhov (R), M. Aeschlimann (CH), J.-Y. Bigot (F), R.D. Coalson (USA), H. Girault (CH), M. Gruebele (USA), J.-E. Moser (CH), A. Rebane (USA), Y.Tanimura (J), M. Wulff (F)

For further information and registration forms:

Dr Marcia T. Portella-Oberli

Inst. de Physique Experimentale,

Faculty des Sciences, BSP

University of Lausanne

1015 Lausanne-Dorigny

tel.: xx-41-21-692 3676 fax: xx-41-21-692 3635

email: QD@ipe.unil.ch also available on the web site: <http://www.unil.ch/ipe/>

5. GORDON RESEARCH CONFERENCE MOLECULAR ELECTRONIC SPECTROSCOPY AND DYNAMICS

Queens College, Oxford, UK, Aug. 31 - Sept. 5, 1997

The 1997 Gordon Research Conference on Molecular Electronic Spectroscopy and Dynamics will be held at Queens College, Oxford, England from August 31 - September 5, 1997, on the High Street. In keeping with the international venue, and the traditions of the meeting, a wide variety of topics relating to electronic spectroscopy and its applications to studies of molecular structure and dynamics in both the gas phase and the condensed phase will be discussed. An active social program also is planned. Program details, application procedures, and travel and accommodation information will be provided at a later date.

David W. Pratt (Chair; pratt+@pitt.edu), Robert W. Field (Vice-Chair; rwfield@mit.edu), John P. Simons (Chair. Local Organizing Committee; jpsimons@vax.ox.ac.uk).

6. Symposium on Dynamics in Molecular Systems

214th ACS National Meeting in Las Vegas, Nevada September 7 - 11, 1997

Tim Zwier and I are organizing a special Symposium at the Las Vegas ACS Meeting. The symposium will run for four days, September 8 - 11, with morning and afternoon oral sessions, and one or two poster sessions. There are seven different sessions listed below with the invited speakers, who have agreed to attend:

PHOTODISSOCIATION

Keiji Morokuma, Alberto Beswick, Hanna Reisler and Fleming Crim.

REACTION DYNAMICS AND COHERENT CONTROL

Herschel Rabitz, Robert Gordon, Jim Valentini and Joel Bowman.

IONS

John Maier, Rob Continetti, Peter Hackett and Kent Ervin.

INTRA- INTERMOLECULAR PROCESSES

Tom Rizzo, Bob Field, Marek Zgierski and Hai-Ping Cheng.

CLUSTERS

Peter Felker, Birgitta Whaley, Dan Neumark, Will Castleman, Ken Leopold, Friedrich Huisken, Stephen Gray and Sherwin Singer.

SURFACES AND SOLIDS

Manfred Kappes, Phillipe Guyot-Sionnest, Barbara Garrison and Ara Apkarian.

We plan to have a number of contributed oral presentations in addition to the invited speakers. If you would like to participate in the Symposium, please send a completed ACS Abstract Form to:

Prof. James M. Lisy Department of Chemistry, Box 7-6 University of Illinois at Urbana-Champaign 600 S. Mathews Ave. Urbana, IL 61801

If you need an abstract form, please contact me by e-mail: j-lisy@uiuc.edu or by telephone: 217-333-2898.

There are a limited number of graduate student travel fellowships (up to \$300) to offset conference fees, travel or local expenses. Please direct these applications (Abstract Form and Supporting Letter indicating our Symposium) to:

Dr. Ellen Stechel, Program Chair Sandia National Laboratories P.O. Box 5800 MS-1421 Albuquerque, NM 87185-1421

We hope to see you in Las Vegas. Don't forget to bring your favorite good luck charm(s).

7. THEORETICAL CHEMISTRY

University of Sussex, Brighton, U.K., 5th December 1997

A one-day meeting has been organised to celebrate the contribution Professor J.N. Murrell has made to Theoretical Chemistry. The programme will consist of contributions from former students, including P. Madden, J. Tennyson, D. Clary, D. Bosanac, A. Varandas, and H. Guo, and will be followed by dinner in the evening. Friends and former colleagues wishing to attend should contact Prof. A.J. Stace, School of Chemistry, Physics and Environmental Science, University of Sussex, Falmer, Brighton BN1 9QJ, U.K.

8. Faraday Division, Royal Society of Chemistry - Faraday Discussion 108 "The Dynamics of Electronically-Excited States in Gaseous, Cluster and Condensed Media"

University of Sussex, UK, 15-17 December 1997

Organising Committee: G S Beddard, R J Donovan, R Grice, J M Hutson, A Orr-Ewing, B Soep, A J Stace, J C Whitehead (Chairman)

There are now a wide range of experiments being performed that can study various aspects of the dynamics of electronically-excited states in gaseous, cluster and condensed phases. The aim of the Discussion will be to explore the similarities and differences between these processes in the different media focusing on the effect of the medium. The processes involved include energy transfer processes, chemical reaction, decomposition to neutral and ionic fragments, proton and electron transfer. Contributions are invited for consideration by the Organising Committee. Titles and abstracts should be submitted by 20th DECEMBER 1996 to Dr J C Whitehead, Chemistry Department, Manchester University, Manchester, M13 9PL (j.c.whitehead@man.ac.uk). Full papers for publication in the Faraday General Discussion 108 will be required by August 1997. Further details about the Discussion can be obtained from Ms Shazia Riaz, riazs@rsc.org.

9. Faraday Division, Royal Society of Chemistry - Faraday Discussion 110 "CHEMICAL REACTION THEORY"

University of St Andrews, Scotland, 1-3 July 1998

CALL FOR ABSTRACTS

This will be the first Faraday Discussion devoted purely to the theory of chemical reactions, one of the most rapidly developing areas of theoretical chemistry. Predictions on the dynamics of the reactions of small molecules can now be as reliable as experimental measurements and the accuracy of calculations on more complicated problems ranging from reactions of organic molecules to reactions on surfaces and in solution is improving at a very fast pace.

The committee specially welcomes theoretical or computational papers in the following areas:

* ab initio calculation of accurate potential energy surfaces for chemical reactions
scattering theory for the accurate treatment of the reactions of small molecules
extension of theory to dynamics and kinetics of larger molecules
reactions of molecules on solid surfaces and in solution

The papers chosen for the Discussion will be concerned with theory or calculations that can be tested by comparison with experiment. St Andrews University on the east coast of Scotland is over 500 years old and is a beautiful place to hold the meeting (especially in July). The accommodation facilities there are excellent. There are good connections to St Andrews from the international airport at Glasgow and also from Edinburgh. Contributions are invited for consideration by the Organising Committee. Titles and abstracts of about 300 words should be submitted no later than 1 JUNE 1997 to Professor D C Clary, Department of Chemistry, University College London, London WC1H OAJ (email: d.c.clary@ucl.ac.uk). Full papers for publication in the Faraday General Discussion 110 volume will be required by February 1998. Organising Committee: D C Clary (Chairman), J N L Connor, I H Hillier, S Holloway, W C Mackrodt, D E Manolopoulos, M A Robb

10. 15th International Symposium on Gas Kinetics

The 15th International Symposium on Gas Kinetics will be held in Bilbao, Spain, during the week 12-19th September 1998. Further details from Prof. F. Castano (qfpcaalf@lgdx02.lg.ehu.es)